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GENDEX--RAT MODULE FOR CONSTRUCTING TREND-FREE FRACTIONAL FACTORIAL AND RESPONSE SURFACE TREATMENT DESIGNS

By

Walter T. Federer
Department of Biometrics, Cornell University;

Nam-Ky Nguyen
Designcomputing,

and

Sophonie Nshinyabakobeje
Department of Biometrics, Cornell University

ABSTRACT

The RAT module of the Gendex toolkit is a program for ordering n treatment combinations (runs) in such a manner as to have them orthogonal or nearly-orthogonal to linear and quadratic time trends. The number of runs at each time point may vary from 1 to n. Four options of model selection are available, i.e., Main-effects model, Interaction model, Full model (quadratic terms of levels of variables added to the Interaction model), and Full model (main-effects are important). Any treatment design or other input may be used for the input design. The program adds the linear and the quadratic standardized orthogonal polynomial regression values. Several example are presented to illustrate various aspects of the RAT program.

Keywords: Main-effect, Interaction, Full model, Orthogonal, Combinations, Linear time trend, Quadratic time trend.

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INTRODUCTION

In various types of investigations, the combinations of a factorial, a fractional replicate of a factorial, a response surface, or other treatment design may be run sequentially through time. There may be a trend, linear or quadratic, through time. The RAT (robust against trend) is a program for arranging the combinations of a treatment design in such a manner as to have the treatment effects orthogonal or nearly orthogonal to the time trends. The algorithm which implements this approach is patterned after the one used for the NOA algorithm (Nguyen, 1996a, 1996b; Federer, Nguyen, and Nshinyabakobeje, 2001). The following briefly describes the approach used for RAT.

. The u^{th} row of the extended design matrix **X**, **W**, for n runs with m_0 (1 or 2 for either linear or linear plus quadratic trends) columns representing the time trends, involving p - m - 1 parameters (p the number of parameters is the number of time trends plus 1 for the mean plus m for the variables of the input design) is $(z_{u1}, \ldots, z_{um0}, 1, x_{u1}, \ldots x_{um}, \ldots, x_{u(p-m0-1)})$. The trend variable z_{uw}, w = 1, 2 is a variable taking on the standardized values of the orthogonal polynomial coefficients for linear and quadratic trends. The runs should be allocated to the time trends such that trend variables and x-variables are orthogonal. For an orthogonal trend design, the inclusion of trends does not affect the estimated regression coefficients of the x-variables and as such the only effect of trends is reducing experimental error. **W** is partitioned as [**Z**|**X**]. Let $\mathbf{M} = \mathbf{W'W}$. **M** can then be partitioned as $\mathbf{M}_{11} = \mathbf{Z'Z}$, $\mathbf{M}_{12} = \mathbf{Z'X}$, $\mathbf{M}_{21} = \mathbf{X'Z}$, and $\mathbf{M}_{22} = \mathbf{X'X}$. The condition for the columns of **X** to be trend free to the columns of **Z** is $\mathbf{Z'X} = \mathbf{0}$.

The approach of RAT to construct a trend free ordering of the combinations (treatments) is to find a suitable ordering of the n combinations (runs)such that the objective function f is minimized where f is the sum of squares of the elements of **Z'X**. Several examples are given to illustrate various aspects of using the RAT module.

USING RAT

To use the RAT module, we assume that it has been placed in the C:\Gendex directory as described by Federer, Gross, Nguyen, and Nshinyabakobeje (2001). The following steps describe how to create a trend free or nearly trend free arrangement of the n runs of the input design:

1. Open the DOS directory. Use CD\Gendex to change the directory from WINDOWS to the C:\Gendex> directory, return.
2. Type notepad to open a notepad file, return.
3. In the open file of notepad either type or paste in the desired treatment design.
4. Save this design in the C:\Gendex directory as rat. The file is saved as rat.txt. Exit notepad.
5. After the prompt C:\Gendex>, type java -cp C:\Gendex Rat, return. (Note that RAT is case sensitive and must be entered in this form. The other terms in the command are not case sensitive.)
6. From the menu and the C:\Gendex directory, highlight the file rat.txt and select open.

7. At the prompt "rat.txt has n rows and m columns?" select YES if correct and NO if not.
8. At the prompt "Choose the number of points at each time point:", select a number from 1 to n to determine the number of runs for each time point. Then click OK.
9. At the prompt "Choose a trend:", select from either linear or quadratic and click OK. Selecting quadratic creates both linear and quadratic trend regressions.
10. At the prompt "Choose a model:", There are four options, Main-effect model, Interaction model, Full model, and Full model (main-effects more important). Select a model and click OK.
11. At the prompt "Enter a random seed:", either enter a number or leave blank. Click OK.
12. At the prompt "Enter the number of tries:", either enter a number or leave blank. Click OK.
13. When the design appears on the screen, click on OK at bottom of screen to save this output as RAT.HTM. A description of the design appears along with the prompt C:\Gendex>. Another design may not be constructed. If Ok is not clicked at bottom of screen, use CONTROL C to return to C:\Gendex>.
14. To obtain a printed copy of RAT.HTM, go to WINDOWS EXPLORER, open the C:\Gendex directory. Highlight the file RAT.HTM. Right click on mouse and select REFRESH. Then open RAT.HTM and select PRINT under FILE.
15. If the file RAT.HTM is to be pasted in a document for editing or copying, highlight the file RAT.HTM. Under EDIT, click on SELECT ALL and then on COPY. Close file and go to document where the content of RAT.HTM is to be copied.

OUTPUT FROM RAT MODULE

The contents of the output from RAT are:
The values of m the number of variables in the input design, $p = m + 1 + m_0$, n the number of runs or treatment combinations, and m_0 the number of time trends are given.
try # indicates the number of tries used to obtain the design.
seed is the number selected for the random seed.
# of iterations is the number of iterations used on the last try to obtain the design.
det is the value of the determinant of **X'X**.
std. Det
TF is one for orthogonal (trend free) designs and less than one otherwise.
Factor levels (columns m_0 to $m_0 + m$ are the columns of the input design)
X'X
inverse(**X'X**) is the inverse of the **X'X** matrix.

EXAMPLES

Example 1. A 2^3 factorial treatment design with the 0 level replaced with -1 is used as the input file which was typed in an open file of C:\Gendex> notepad, return. There are m = 3 factors (A, B, and C) and p = 5 parameters. The parameter vector is **B** = [linear regression mean A B C]. The object is to create an ordering of the runs (combinations) which is orthogonal or nearly orthogonal to the trend parameters. The steps used to obtain the output was:

1. In an open notepad file, type the n = 8 combinations of the 2^3 factorial with a -1 replacing the 0. SAVE this file as rat in the C:\Gendex directory. Close notepad.
2. At the prompt C:\Gendex>, type java -cp C:\Gendex Rat, return. (Note Rat must be typed in this form as the program is case sensitive but only for this term.).
3. When the MENU appears, from the C:\Gendex directory, highlight the file rat.txt and click on OPEN.
4. At the prompt, "rat.txt has 8 rows and 3 columns?", click on YES.
5. At the prompt, "Choose the number of points at each level:", 1 was selected.
6. At the prompt, "Choose a trend:", linear was selected.
7. At the prompt, "Choose a model:", Main-effect model" was selected.
8. At the prompt, "Enter a random seed", this was left blank and OK was clicked on.
9. At the prompt, "Enter the number of tries", this was left blank and OK was clicked on.
10. When the output appeared on the screen, OK at the bottom of the screen was clicked on.
11. In WINDOWS EXPLORER and the C:\Gendex directory, the file RAT>HTM (usually at the bottom of the files) was highlighted. Then, right click on mouse was used to select REFRESH. The file RAT.HTM was highlighted and under FILE, OPEN was selected. Under EDIT, SELECT ALL was highlighted and then COPY. The file was closed.
12. In the word processing program MICROSOFT WORD, the following output was pasted. (Some realignment was necessary to obtain this form.)

RAT 1.1: construct trend-free fractional factorial and response surface designs
(C) 2001 Design Computing (URL: http://designcomputing.hypermart.net/gendex)

Note: design for m=3, p=5, n=8 and m0=1.

try #	1
seed	1010512031620
# of iterations	3
f	0
det	14043.42857142857
std. det	0.42857143
TF	1

Factor levels (columns 2-4):

-1	-1	-1	-1
-0.7143	1	1	1
-0.4286	-1	1	1
-0.1429	1	-1	-1
0.1429	1	-1	1
0.4286	-1	1	-1
0.7143	1	1	-1
1	-1	-1	1

X'X

3.4286	0	0	0	0
	8	0	0	0
		8	0	0
			8	0
				8

inverse(X'X)

0.2917	0	0	0	-0
	0.125	0	0	-0
		0.125	0	-0
			0.125	-0
				0.125

Note: RAT used 0.11 seconds.

The **X** matrix is

-1	1	-1	-1	-1
-0.7143	1	1	1	1
-0.4286	1	-1	1	1
-0.1429	1	1	-1	-1
0.1429	1	1	-1	1
0.4286	1	-1	1	-1
0.7143	1	1	1	-1
1	1	-1	-1	1

The input design is the last three columns of the **X** matrix. The program inserts the orthogonal polynomial linear regression coefficients. The second column of ones is for the mean. The **X'X** matrix is diagonal and the diagonal elements are the sums of squares of the elements of the columns of **X**. The value for f is 0 since all off-diagonal elements in the first row of **X'X** are zero and the ordering is trend free. The value of the determinant is $3.4286 \times 8 \times 8 \times 8 \times 8 = 14{,}043.5457$. The value for TF (trend free) is 1 since this is an orthogonal design.

Example 2. The same input design of a 2^3 factorial is used here. The only difference is that the Interaction model was selected. The output obtained was:

RAT 1.1: construct trend-free fractional factorial and response surface designs
(C) 2001 Design Computing (URL: http://designcomputing.hypermart.net/gendex)

Note: design for m=3, p=8, n=8 and m0=1.

try #	1
seed	1010512488000
# of iterations	2
f	6.53
det	5478274.612244898
std. det	0.3265306
TF	0.9619

Factor levels (columns 2-4):

-1	-1	1	1
-0.7143	-1	-1	-1
-0.4286	1	-1	1
-0.1429	1	1	-1
0.1429	1	-1	-1
0.4286	-1	1	-1
0.7143	1	1	1
1	-1	-1	1

X'X

3.4286	-0	0.5714	0	0.5714	1.7143	0	-1.7143
	8	0	0	0	0	0	0
		8	0	0	0	0	0
			8	0	0	0	0
				8	0	0	0
					8	0	0
						8	0
							8

inverse(X'X)

0.3828	0	-0.0273	-0	-0.0273	-0.082	-0	0.082
	0.125	-0	-0	-0	-0	-0	0
		0.127	0	0.002	0.0059	0	-0.0059
			0.125	0	0	0	-0
				0.127	0.0059	0	-0.0059
					0.1426	0	-0.0176
						0.125	-0
							0.1426

Note: RAT used 0.11 seconds.

The **X** matrix is obtained by adding three columns to the **X** matrix of Example 1. The product of coefficients in columns 3 and 4, in columns 3 and 5, and in columns 4 and 5 make up these last three columns. The parameter vector is **B** = [linear regression mean A B C AB AC BC]. The mean, B, and AC are orthogonal to the linear trend. The A effect is partially confounded with C, AB, and BC. The C effect is partially confounded with AB and BC. The AB effect is partially confounded with the BC effect. This partial confounding of effects with the linear trend is the reason that TF = 0.9619 instead of 1. The value for f is obtained as $0 + 0.5714^2 + 0.5714^2 + 0 + (-1.7143)^2 + (-1.7143)^2 = 6.53$.

Example 3. Using the same 2^3 factorial design input as for previous examples, the only difference with the last example is that the Full model was selected rather than the Interaction model. The output obtained was:

RAT 1.1: construct trend-free fractional factorial and response surface designs
(C) 2001 Design Computing (URL: http://designcomputing.hypermart.net/gendex)

Note: design for m=3, p=8, n=8 and m0=1.

try #	1
seed	1010512669420
# of iterations	1
f	6.53
det	5478274.6122448975
std. det	0.3265306
TF	0.9619

Factor levels (columns 2-4):

-1	-1	1	-1
-0.7143	1	1	1
-0.4286	-1	-1	1
-0.1429	1	-1	-1
0.1429	1	1	-1
0.4286	-1	1	1
0.7143	1	-1	1
1	-1	-1	-1

X'X

3.4286	0	-0	-2.2857	-0	-0	-0	1.1429
	8	0	0	0	0	0	0
		8	0	0	0	0	0
			8	0	0	0	0
				8	0	0	0
					8	0	0
						8	0
							8

inverse(X'X)

0.3828	-0	0	0.1094	0	0	0	-0.0547
	0.125	-0	-0	-0	-0	-0	0
		0.125	0	0	0	0	-0
			0.1562	0	0	0	-0.0156
				0.125	0	0	-0
					0.125	0	-0
						0.125	-0
							0.1328

Note: RAT used 0.27 seconds.

As may be noted from the **X'X** matrix there is less confounding of effects for the Full model than for the Interaction model. The parameter vector and **X** matrix are the same as for the Interaction model.

Example 4. To illustrate the output for the Full model (main effects more important), we use the same 2^3 factorial input design as above. The output obtained was:

RAT 1.1: construct trend-free fractional factorial and response surface designs
(C) 2001 Design Computing (URL: http://designcomputing.hypermart.net/gendex)

Note: design for m=3, p=8, n=8 and m0=1.

try #	2
seed	2017721452
# of iterations	3
f	6.53*
det	5478274.612244897
std. det	0.3265306
TF	0.9619

Factor levels (columns 2-4):

-1	1	-1	-1
-0.7143	1	1	1
-0.4286	-1	-1	1
-0.1429	-1	1	-1
0.1429	-1	1	1
0.4286	-1	-1	-1
0.7143	1	1	-1
1	1	-1	1

X'X

3.4286	0	0	-0	-0	-0	1.1429	-2.2857
	8	0	0	0	0	0	0
		8	0	0	0	0	0
			8	0	0	0	0
				8	0	0	0
					8	0	0
						8	0
							8

inverse(X'X)

0.3828	-0	-0	0	0	0	-0.0547	0.1094
	0.125	0	-0	-0	-0	0	-0
		0.125	-0	-0	-0	0	-0
			0.125	0	0	0	0
				0.125	0	-0	-0
					0.125	-0	0
						0.1328	-0.0156
							0.1562

Note: RAT used 0.33 seconds.

In the above X'X matrix, note that the A, B, C, and AB effects are orthogonal to a linear trend.

Example 5. Using a 2^4 factorial design as the input file of n = 16 runs (combinations), linear and quadratic trends, the Full model option was selected. Also as before, the number of points at each level was 1. The output obtained was:

RAT 1.1: construct trend-free fractional factorial and response surface designs
(C) 2001 Design Computing (URL: http://designcomputing.hypermart.net/gendex)

Note: design for m=4, p=13, n=16 and m0=2.

try #	1
seed	1010592749690
# of iterations	7
f	28.28
det	3.5136655378494406E14
std. det	0.078019045
TF	0.9692

Factor levels (columns 3-6):

-1	1	1	1	1	1
-0.8667	0.6	1	-1	1	-1
-0.7333	0.2571	-1	-1	-1	1
-0.6	-0.0286	-1	1	-1	-1
-0.4667	-0.2571	1	1	-1	-1
-0.3333	-0.4286	1	-1	-1	1
-0.2	-0.5429	-1	-1	1	-1
-0.0667	-0.6	-1	1	1	1
0.0667	-0.6	1	1	1	-1
0.2	-0.5429	1	-1	1	1
0.3333	-0.4286	-1	-1	-1	-1
0.4667	-0.2571	-1	1	-1	1
0.6	-0.0286	1	1	-1	1
0.7333	0.2571	1	-1	-1	-1
0.8667	0.6	-1	-1	1	1
1	1	-1	1	1	-1

X'X

6.0444	-0	0	-2.1333	0	-0	0	-1.0667	-4.2667	-0	-0	0	-0
	4.6629	0	0	0.4571	1.8286	-0	0	0	-0	0.9143	0	0
		16	0	0	0	0	0	0	0	0	0	0
			16	0	0	0	0	0	0	0	0	0
				16	0	0	0	0	0	0	0	0
					16	0	0	0	0	0	0	0
						16	0	0	0	0	0	0
							16	0	0	0	0	0
								16	0	0	0	0
									16	0	0	0
										16	0	0
											16	0
												16

inverse(X'X)

0.2197	0	-0	0.0293	-0	0	-0	0.0146	0.0586	0	0	-0	0
	0.2279	-0	-0	-0.0065	-0.026	0	0	0	0	-0.013	-0	0
		0.0625	-0	0	0	-0	-0	-0	-0	0	0	-0
			0.0664	-0	0	-0	0.002	0.0078	0	0	-0	0
				0.0627	0.0007	-0	-0	-0	-0	0.0004	0	-0
					0.0655	-0	0	0	-0	0.0015	-0	0
						0.0625	-0	-0	-0	-0	0	-0
							0.0635	0.0039	0	0	-0	0
								0.0781	0	0	-0	0

0.0625	-0	-0	0
	0.0632	-0	0
		0.0625	-0
			0.0625

Note: RAT used 0.33 seconds.

Example 6. Using the same set-up as Example, 2 points instead of 1 are selected for each of 4 time points (# of time points not indicated in output but can be obtained under factor levels). The output obtained was:

RAT 1.1: construct trend-free fractional factorial and response surface designs
(C) 2001 Design Computing (URL: http://designcomputing.hypermart.net/gendex)

Note: design for m=3, p=5, n=8 and m0=1.

try #	1
seed	1010594676260
# of iterations	2
f	0
det	18204.444444444445
std. det	0.5555556
TF	1

Factor levels (columns 2-4):

-1	-1	-1	-1
-1	1	1	1
-0.3333	-1	-1	1
-0.3333	1	1	-1
0.3333	-1	1	1
0.3333	1	-1	-1
1	-1	1	-1
1	1	-1	1

X'X

4.4444	0	0	0	-0
	8	0	0	0
		8	0	0
			8	0
				8

inverse(X'X)

0.225	0	0	-0	0
	0.125	0	0	-0
		0.125	0	-0
			0.125	-0
				0.125

Note: RAT used 0.22 seconds.

Example 7. Using a 3^2 factorial as the input design, selecting linear trend, selecting one level at each time point, and selecting the Full model, the following output was obtained:

RAT 1.1: construct trend-free fractional factorial and response surface designs

Note: design for m=2, p=7, n=9 and m0=1.

try #	1
seed	1010595253740
# of iterations	6
f	0
det	19440.0
std. det	0.004064421
TF	1

Factor levels (columns 2-3):

-1	1	0
-0.75	-1	1
-0.5	0	-1
-0.25	-1	-1
0	0	0
0.25	1	1
0.5	0	1
0.75	1	-1
1	-1	0

X'X

3.75	0	0	0	0	0	0
	9	0	0	0	6	6
		6	0	0	0	0
			6	0	0	0
				4	0	0
					6	4
						6

inverse(X'X)

0.2667	0	0	0	0	0	-0
	0.5556	0	0	0	-0.3333	-0.3333
		0.1667	0	0	0	-0
			0.1667	0	0	-0
				0.25	0	-0
					0.5	-0
						0.5

Note: RAT used 0.05 seconds.

The parameter vector **B** = [linear regression mean AL BL AL*BL AQ BQ], where VL (V = A or B) is the regression for linear trend and VQ is the regression for quadratic trend. In the **X** matrix, the columns for AQ and BQ are obtained as the squared coefficients in columns 3 and 4, column 2 being a column of ones for the mean.

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